REVIEW OF DIATOMIC SPECTROSCOPIC DATA

LAURA K McKEMMISH, *School of Chemistry, University of New South Wales, Sydney, NSW, Australia.*

Accurate and comprehensive diatomic molecular spectroscopic data have long been crucial for measuring and monitoring gaseous environments, e.g. astrophysically, as well as for benchmarking theoretical approaches and, increasingly in ultracold physics. Theory and experiment can be used independently or together to produce useful data that can be highly detailed (e.g. line lists) or summative (e.g. molecular constants).

Accessing these data can be challenging; when data is compiled, knowing the right database can be sufficient, but in many cases data is not compiled or is severely out of data and manual literature searching and data extraction is thus required.

Here, I will summarise my recent review of diatomic spectroscopic data (WIREs Comput Mol Sci. 2021;E1520). I will summarise the key diatomic data types and their interconnectivity. I will also provide strategies to strengthen the connection between data producers (e.g. ab-initio electronic structure theorists and experimental spectroscopists), data modellers (e.g. line list creators) and data users (astronomers, chemical physicists, etc). A particular focus is ensuring that new data is optimally utilised with appropriate attribution.